

SELF-ASSEMBLED MONOLAYER OF ENGINEERED ORGANIC MOLECULES FOR MOLECULAR ELECTRONICS

Govind Mallick, Anubhav Srivastava, Sarah Lastella and Shashi P. Karna

Army Research Laboratory
Weapons and Materials Research Directorate,
ATTN: AMSRD-ARL-WM-BD
Aberdeen Proving Grounds, MD 21005-5069

Qingdon Zheng and Paras N. Prasad
Institute for Lasers, Photonics, and Biophotonics
The University at Buffalo
450 Natural Science and Mathematics Complex
Buffalo, NY 14260

Alma E Wickenden and Madan Dubey
US Army Research Laboratory
Sensors and Electron Devices Directorate
ATTN: AMSRD-ARL-SE-RL
2800 Powder Mill Road
Adelphi, MD 20783

ABSTRACT

A series of molecules for applications in molecular electronics were modeled, synthesized, and self-assembled on a thin Au film on lightly doped Si. The atomic force microscopy of the assembled molecules exhibits uniform distribution.

molecules at the Au surface in the “hollow” spaces has also been reported by other authors.³ Details of the modeling, synthesis, SAM preparation, and characterization of the electrical and surface properties will be presented in a later paper.

SUMMARY

A challenge in realizing molecular-scale devices is the lack of appropriate molecular architecture and controlled assembly of molecules on a solid substrate. Self-assembled monolayers provide a uniform hierarchical structure for developing molecular-scale electronic and sensor devices.^{1,2} As a part of our joint efforts to develop materials, assembly techniques, and understanding of the basic device physics, we have modeled a series of molecular structures by quantum mechanical calculations. The related structures have been synthesized and self-assembled on thin Au films on Si substrates. One of the structures shown in Figure 1, exhibited excellent self-assembly properties at a concentration of 1.135×10^{-3} M in tetrahydrofuran (THF) solution. The self-assembled monolayers (SAM) exhibited reproducible uniformity, as shown in the atomic force microscope (AFM) image (Figure 2). Lower concentrations did not exhibit this self-assembly property under identical conditions. Analysis of the AFM image suggests that the molecules prefer to attach in the (hollow) space surrounded by three Au atoms. This preferential binding of organic

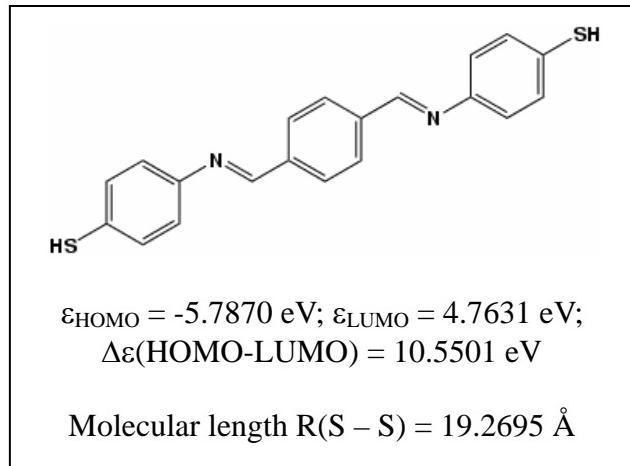


Figure 1. *Ab initio* optimized geometry and energy (ϵ) for highest occupied (HO) and lowest unoccupied (LU) molecular orbitals

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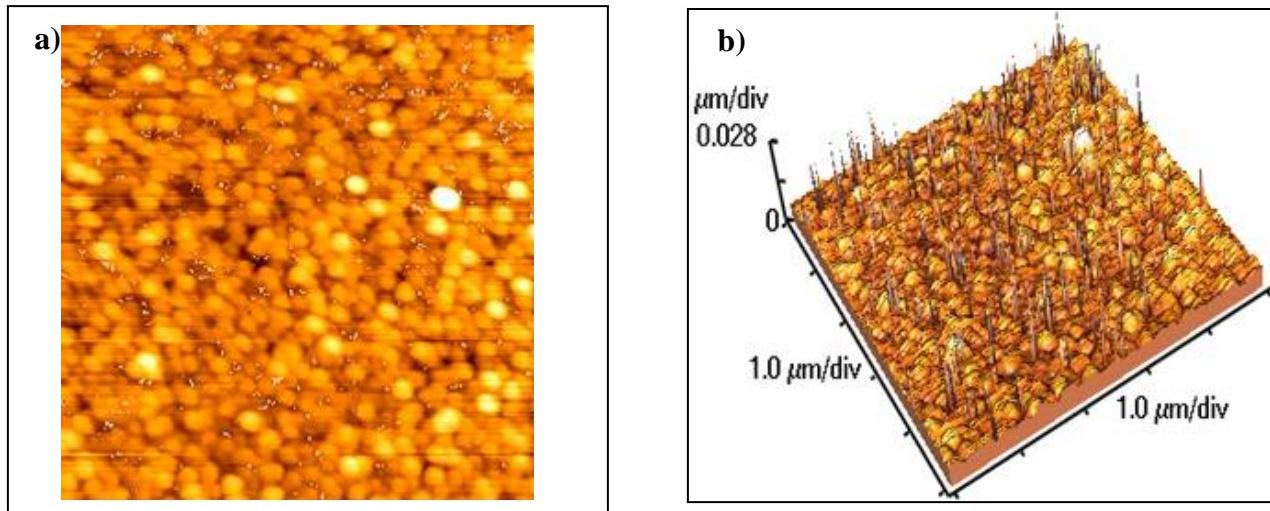


Figure 2: (a) 2-D AFM $1 \times 1 \mu\text{m}^2$ image of ME3 SAM on Au film. White dots represent the molecules attached at the Au surface. (b) 3-D AFM image of (a). The vertical

peaks correspond to the assembled molecular bundles, having an average height of $\sim 2 \text{ nm}$.

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